

Thermal hydrologic model of permafrost

1.0 Model formulation

The non-isothermal dynamics of water in porous media above and below the freezing temperature is considered. A nonisothermal, two-component, three-phase model was presented by Painter [2011]. Here this model is simplified to a single component (water in the ice, liquid and vapor phases) and an energy balance. The approach is equivalent to a temperature dependent version of Richards equation with an option to partition to the ice phase.

1.1 Conservation equations

Using the extended Darcy's law for multiphase flow, the conservation equation for water is written

$$\frac{\partial}{\partial t} \left[\sum_{p=l,g,i} \phi \omega_p n_p s_p \right] = - \sum_{p=l,g} \nabla \cdot [\omega_p n_p \mathbf{V}_p] + \nabla \cdot [\phi s_g \tau_g n_g D_g \nabla \omega_g] + Q \quad (1)$$

where the Darcy velocity \mathbf{V}_p is defined by

$$\mathbf{V}_p = - \frac{k_r k}{\mu_p} (\nabla P_p + \rho_p g \nabla z) \quad (2)$$

Here s is the phase saturation ($s_l + s_g + s_i = 1$), t is time, ϕ is porosity, n is density on a molar basis, ρ is mass density, ω is mole fraction of water, k is the absolute permeability, k_r is relative permeability, μ is dynamic viscosity, z is the vertical coordinate, g is the acceleration due to gravity, D is the diffusion coefficient, Q is the mass source rate, and τ is the phase-dependent tortuosity. Note the phase saturation is included in the diffusion term, which differs from that of Painter [2011]. That work included the saturation in the tortuosity. The subscripts l , g , and i represent liquid, gas and ice phases, respectively. Ice-phase air and dissolved air are ignored, so $\omega_i = 1$ and $\omega_l = 1$.

Setting the gas pressure to the hydrostatic condition eliminates the gas advection term from eq 1. In addition, the constraint that the vapor pressure be equal to the saturated vapor pressure can be used to rewrite the $\nabla \omega_g$ term

$$\nabla \omega_g = \nabla \left(\frac{p_v}{p_g} \right) = \nabla \left(\frac{p_{sv}(T)}{p_g} \right) = \frac{1}{n_g R T} \nabla (p_{sv}(T)) = \frac{1}{n_g R T} \frac{\partial p_{sv}}{\partial T} \nabla T \quad (3)$$

where R is the ideal gas constant 461.5 J/kg-K and $p_{sv}(T)$ is the saturated vapor pressure. The water balance equation becomes

$$\frac{\partial}{\partial t} \left[\sum_{p=l,g,i} \phi \omega_p n_p s_p \right] = - \nabla \cdot [\omega_l n_l \mathbf{V}_l] + \frac{1}{R} \nabla \cdot \left[\phi s_g \tau_g D_g \frac{1}{T} \frac{\partial p_{sv}}{\partial T} \nabla T \right] + Q \quad (4)$$

The corresponding energy balance equation assumes local thermal equilibrium

among the ice, liquid, gas and rock, leading to

$$\frac{\partial}{\partial t} \left[\sum_{p=l,g,i} (\phi \rho_p s_p u_p) + (1 - \phi) \rho_{rock} u_{rock} \right] = -\nabla \cdot (\rho_l h_l \mathbf{V}_l) + \nabla \cdot [\kappa_e \nabla T] + H \quad (5)$$

Where T is temperature, u is specific internal energy, h is specific enthalpy, κ_e is the equivalent thermal conductivity for the rock-water-ice mixture, H is the thermal energy source, and the subscript *rock* denotes the solid (rock) phase.

Primary variables are temperature T and liquid pressure p_l . Note that no variable change is required when going from partially saturated to fully saturated conditions. However, the situation of full dryout $s_g = 1$ is not allowed.

1.2 Constitutive Relationships

1.2.2 Saturation/pressure relationships

Functional relations between phase saturations and interphase capillary pressures are required. In partially frozen geological material, water is generally the wetting phase with respect to both air and ice, implying that ice forms first in the largest water-filled pores. It is also generally assumed that a thin film of water separates the ice from gas and prevents a direct gas-ice interface. Thus, two retention curves (saturation-capillary pressure relations) are required, one for the ice-liquid pair and one for the liquid-gas pair.

In multiphase systems, the retention curves for all phase pairs can be related to the retention curve for any two-phase system by an interfacial-tension dependent rescaling of the capillary pressure [14]. For the ice-water-gas system,

$$\frac{s_l}{s_l + s_i} = S_* \left(\frac{\sigma_{gl}}{\sigma_{il}} P_{cil} \right) \quad (6)$$

$$\frac{s_l}{s_l + s_g} = S_* \left(P_{cgl} \right) \quad (7)$$

where S_* is the retention curve for the two-phase system with unfrozen liquid and gas, σ_{gl} and σ_{il} are gas-liquid and ice-liquid interfacial tensions, P_{cgl} is the gas-liquid capillary pressure ($p_g - p_l$) and P_{cil} is the ice-liquid capillary pressure ($p_i - p_l$). The left side of equation 6 is the “unfrozen fraction” and the left side of equation 7 is the “apparent” liquid saturation (ratio of unfrozen liquid to available pore space). For clarity, the residual (irreducible) liquid saturation has been set to zero, but this can easily be included.

The ice-liquid capillary pressure is understood to be determined by the temperature and chemical composition of the liquid phase, independent of the liquid water content [15]. Grant and Sletten [15] review several derivations and recommend the development of Brun et al. [16] as the most rigorous. The expressions reviewed by Grant and Sletten are all within 10% of the Brun et al. [16] expressions over the temperature range 230-273 K. At lower temperatures, the relative differences can be larger, but the unfrozen fraction is negligible at those temperatures, and the absolute error incurred by using the more approximate expression in the calculation of unfrozen fraction is too small to have any

meaningful effect. Because of this insensitivity to the exact representation, Loch's model [17]

$$P_{cil} = -\rho_i h_{iw}^0 \ln\left(\frac{T}{T_0}\right) \quad (8)$$

is approximated as

$$P_{cil} = \rho_i h_{iw}^0 \frac{T_0 - T}{T_0} \quad (9)$$

Here h_{iw}^0 is the heat of fusion of water at $T_0 = 273.15$ K.

Several empirical forms exist for the soil moisture retention curve S_* . Van Genuchten's [18] model has been successful for a wide range of media and is widely used.

$$S_*(P_c) = \left[1 + \left(\frac{P_c}{P_0}\right)^\nu\right]^{-\lambda} \quad \text{for } P_c > 0 \quad (10)$$

$$S_*(P_c) = 1 \quad \text{for } P_c \leq 0$$

where P_0 and ν are curve fitting parameters and $\lambda = 1 - 1/\nu$. Note that Eq. 10 does not allow a non-zero air entry pressure but modifications that accommodate a non-zero air entry pressure have been developed [19].

The computational steps in establishing the phase saturations from the primary variables can now be described. Recall that the gas-liquid capillary pressure is always known because liquid pressure is a primary variable and gas pressure is fixed. Similarly temperature and thus ice-liquid capillary pressure are always known. Thus the right sides of 6 and 7 are always known. If $p_l > p_g$ then the

Let $A \equiv \frac{1}{S_*(\gamma T')}$ where $\gamma \equiv \frac{\sigma_{gl}}{\sigma_{il}} \rho_i h_{iw}^0$ and $T' \equiv \frac{T_0 - T}{T_0}$. Also let $B \equiv \frac{1}{S_*(p_g - p_l)}$.

Then

$$s_l = 1/(A + B - 1)$$

$$s_g = s_l(B - 1)$$

$$s_i = s_l(A - 1) = 1 - s_l - s_g$$

Note that if temperature is above the nominal freezing point, $A=1$, the ice saturation is 0 and the liquid and gas saturations are determined purely from the unfrozen moisture retention curve. If the liquid pressure exceeds the gas pressure, $B=1$, $s_g = 0$, and partitioning between the ice and liquid phase is purely a function of temperature through equation 6 with 9.

1.2.3 Relative permeability

Relationships between the liquid and gas relative permeabilities and the phase saturations are also required. The liquid phase relative permeability in MarsFlo is

based on van Genuchten's fit combined with Mualem's [20] model for relative permeability

$$k_{rl} = (s_l)^{1/2} \left[1 - \left(1 - (s_l)^{1/\lambda} \right)^\lambda \right]^2 \quad (12)$$

Because of its low viscosity, the gas phase tends to be highly mobile and the gas-phase relative permeability is generally less important than liquid relative permeability. A simple linear relationship $k_{rg} = s_g$ is used here.

1.2.4 Thermal conductivity

Thermal conductivity in unfrozen soils or rocks is often written as

$$\kappa_e = \kappa_{dry} + (\kappa_{sat,l} - \kappa_{dry}) Ke_u \quad (13)$$

where $Ke_u = Ke_u(s_l)$ is the Kersten number for unfrozen conditions, s_l is the liquid saturation, $\kappa_{sat,l}$ is the liquid-saturated thermal conductivity and κ_{dry} is the dry conductivity.

For soils or rocks that are frozen and with no liquid water content, the corresponding equation is

$$\kappa_e = \kappa_{dry} + (\kappa_{sat,i} - \kappa_{dry}) Ke_f \quad (14)$$

where $Ke_f = Ke_f(s_i)$ is the Kersten number for frozen conditions, s_i is the ice saturation, $\kappa_{sat,i}$ is the thermal conductivity under ice-saturated conditions.

The Kersten numbers in Eq. 13 and 14 are simply ratios of partially saturated thermal conductivity to fully saturated thermal conductivity (e.g. [21]). Both range from 0 for dry conditions to 1 for saturated conditions and are, in general, nonlinear functions of the respective saturation indices. A power-law function is assumed here as a convenient model

$$Ke_u = (s_l + \varepsilon)^{\alpha_u} \quad (15)$$

$$Ke_f = (s_i + \varepsilon)^{\alpha_f} \quad (16)$$

where α_u and α_f are empirical exponents and $\varepsilon \ll 1$ is a regularization parameter that prevents, for numerical reasons, the derivative with respect to s_l or s_i from becoming unbounded at 0 when α_u and α_f are less than 1.

For a general-purpose code, thermal conductivity is needed as a function of both s_l and s_i . To this end, bilinear interpolation in the Kersten numbers is introduced here

$$\kappa_e = Ke_f \kappa_{sat,f} + Ke_u \kappa_{sat,u} + (1 - Ke_f - Ke_u) \kappa_{dry} \quad (17)$$

There are two options for specifying the dry and saturated thermal conductivities: they may be considered empirically determined parameters and directly specified as input or they may be related to the grain conductivity (κ_g) and porosity ϕ .

For saturated conductivity, the following have been proposed [21]

$$\kappa_{sat,u} = \kappa_{mg}^{1-\phi} \kappa_w^\phi \quad (18)$$

and

$$\kappa_{sat,f} = \kappa_{mg}^{1-\phi} \kappa_i^\phi \quad (19)$$

where κ_i , κ_w , κ_{mg} are thermal conductivities for water ice, liquid water, and mineral grains, respectively.

For κ_{dry} , the following empirical fit has been shown to be reasonably accurate [22]

$$\kappa_{dry} = \frac{0.135\rho_b + 64.7}{\rho_{mg} - 0.947\rho_b} \quad (20)$$

where ρ_b and ρ_{mg} are the dry bulk and grain densities, respectively, in kg m^{-3} and κ_{dry} is in $\text{W m}^{-1} \text{K}^{-1}$. This equation is now placed in a more convenient form. Using $\rho_b = \rho_{mg}(1 - \phi)$, and imposing the constraints that κ_{dry} equal the thermal conductivity of air (κ_a) and the mineral grain thermal conductivity (κ_{mg}) when porosity is 100% and zero, respectively, results in

$$\kappa_{dry} = \frac{d(1 - \phi)\kappa_{mg} + \kappa_a\phi}{d(1 - \phi) + \phi} \quad (21)$$

where d is 0.053 (unitless).

1.2.5 Diffusion coefficients

The binary diffusion coefficient is adjusted for temperature and pressure as [24]

$$D_{12} = D_{12}^0 \left(\frac{P_{ref}}{P} \right) \left(\frac{T}{T_{ref}} \right)^{1.8} \quad (23)$$

where D_{12}^0 is the value at reference temperature and pressure conditions and temperature is in Kelvin.

The phase-dependent tortuosity is written in the form

$$\tau_g = \tau_0 \phi^{\beta-1} s_g^{\beta'-1} \quad (25)$$

β and β' are empirical parameters. The Millington-Quirk model [26] for gas-phase tortuosity is recovered by setting $\beta_g = 4/3$ and $\beta'_g = 10/3$ (check this: $7/3$ or $13/3$?). The parameter τ_0 is a user-specified constant and is typically taken to be unity.

References

Painter, S.L. Three-phase numerical model of water migration in partially frozen geological media: model formulation, validation, and applications
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10.1007/s10596-010-9197-z

1. Perfect, E., Groenevelt, P.H., Kay, B.D.: Transport phenomena in frozen porous media. In Bear, J., Corapcioglu, M.Y. (eds.) *Transport Process in Porous Media*. Kluwer Academic Publishers, Netherlands (1991)
2. Miller, R.D.: Freezing phenomena in soils. In Hillel, D. (ed.) *Application of Soil Physics*. Academic Press, New York (1980)
3. Clifford, S.M.: The role of thermal vapor diffusion in the subsurface hydrological evolution of Mars. *Geophys. Res. Letts.* **18**(11), 2055–2058 (1991)
4. Harlan, R.L.: Analysis of coupled heat-fluid transport in partially frozen soil. *Water Resour. Res.* **9**(5), 1314–1323 (1973)
5. Jame, Y.-W., Norum, D.I.: Heat and mass transfer in freezing unsaturated porous medium. *Water Resour. Res.* **16**(4), 811–819 (1980)
6. Guymon, G.L., Luthun, J.N.: A coupled heat and moisture transport model for arctic soils. *Water Resour. Res.* **10**(5), 915–1001 (1974)
7. Fuchs, M., Campbell, G.S., Papendick, R.I.: An analysis of sensible and latent heat flow in a partially frozen unsaturated soil. *Soil Sci. Soc. Am. J.* **42**(3), 379–385 (1978)
8. Hansson, K., J. Simunek, Mizoguchi, M., Lundin, L.-C., van Genuchten, M.Th.: Water flow and heat transport in frozen soil: Numerical solution and freeze-thaw applications. *Vadose Zone J.* **3**, 693–704 (2004)
9. Panday, S., Corapcioglu, M.Y. Theory of phase-separate multicomponent contaminant transport in frozen soils. *J. Contam. Hyd.* **16**, 235–269 (1994)
10. White, M.D.: Theory and numerical application of subsurface flow and transport for transient freezing conditions, In *Proceedings of the Fifteenth Annual American Geophysical Hydrology Days*, 339–352 (1995)
11. White, M.D., Oostrom, M.: STOMP subsurface transport over multiple phases: Users guide PNNL-15782. Pacific Northwest National Laboratory, Richland, Washington (2006)
12. Pruess, K., Oldenburg, C., Moridis, G.: *Tough 2 User's Guide, Version 2*, LBNL-43134, Lawrence Berkeley National Laboratory, Berkeley, California (1999)
13. Lichtner, P.C. Continuum formulation of multicomponent-multiphase reactive transport. In Lichtner, P.C., Steefel, C.I., Oelkers, E.H. (ed.) *Reactive Transport in Porous Media*. Mineralogical Society of America, Washington DC (1996)
14. Leverett, M.S., Lewis, W.B.: Steady flow of gas-oil-water mixtures through unconsolidated sands. *Trans. AIME, Am. Inst. Min. Metall. Pet. Eng.* **142**, 152–169 (1947)
15. Grant, S.A., Sletten, R.S.: Calculating capillary pressure in frozen and ice-free soils below the melting temperature. *Environ. Geol.* **42**(2), 130–136 (2002)
16. Brun, M., Lallemand, A., Quinson, J-F., Eyraud, C.: A new method for simultaneous determination of the size and shape of pores: The thermoporometry. *Thermochim. Acta* **21**, 59–88 (1977)
17. Loch, J.P.G.: Thermodynamic equilibrium between ice and water in porous media, *Soil Sci.* **126**, 77–80 (1977)
18. van Genuchten, M.Th.: A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. *Soil Sci. Soc. Am. J.* **44**, 892–898 (1980)
19. Vogel, T., van Genuchten, M.Th., Cislerova, M.: Effect of the shape of the soil hydraulic functions near saturation on variably saturated flow predictions. *Adv. Water Resour.* **24**(2), 133–144 (2000)
20. Mualem, Y.: A new model for predicting the hydraulic conductivity of unsaturated porous media. *Water Resour. Res.* **12**, 513–522 (1976)
21. Andersland, O.B. and Ladanyi, B.: *An Introduction to Frozen Ground Engineering*, Chapman and Hall, New York (1994)
22. Peters-Lidard, C.D., Blackburn, E., Liang, X., Wood, E.F.: The effect of thermal conductivity parameterization on surface energy fluxes and temperatures. *J. Atmos.* **55**,

- 1209–1224 (1998)
23. Clifford, S.M., Hillel, D.: Knudsen diffusion: The effect of small pore size and low gas pressure on gaseous transport in soil. *Soil Sci.* 141, 289–297 (1986)
24. Bird, R.A., Stewart, W.E., Lightfoot, E.N.: *Transport Phenomena*, 2nd Edition, John Wiley and Sons, New York (2003)
25. Bear, J.: *Dynamics of Fluids in Porous Media*, Dover Publications, New York (1998)
26. Millington, R.J., Quirk, J.M.: Permeability of porous solids. *Trans. Faraday Soc.* 57, 1200–1207 (1961)
27. Narasimhan, T.N., Witherspoon, P.A.: An integrated finite-difference method for analyzing fluid flow in porous media, *Water Resour. Res.* 12(1), 57–64 (1976)
28. Saad, Y.: *Iterative Methods for Sparse Linear Equations*, 2nd Edition, Society for Industrial and Applied Mathematics, Philadelphia (2003)
29. Mizogouchi, M.: *Water, Heat and Salt Transport in Freezing Soil*. Ph.D. Thesis. (In Japanese) University of Tokyo (1990)
30. Chen, Z., Huan, G., Ma, Y. *Computational Methods for Multiphase Flows in Porous Media*, Society of Industrial and Applied Mathematics, Philadelphia PA (2006)
31. Painter, S.: Three-phase simulations of moisture movement in the Martian subsurface, In *Proceedings of the 9th International Conference on Mars* (2007)
32. Manning, C.E., Ingebritson, S.E.: Permeability of the continental crust: Implications of geothermal data and metamorphic systems, *Rev. Geophys.* 37, 127–150 (1999)
33. Clifford S.M., Parker T.J.: The evolution of the Martian hydrosphere: Implications for the fate of a primordial ocean and the current State of the northern plains, *Icarus* 154, 40-79 (2001)
34. Harrison, K.P., Grimm R.E.: Tharsis recharge: A source of groundwater for Martian outflow channels, *Geophys. Res. Lett.* 31, doi:10.1029/2004GL020502 (2004)